

ON THE STRUCTURE OF BAND EDGES OF 2D PERIODIC ELLIPTIC OPERATORS

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To the memory of Yuri Safarov, our dear friend and colleague

ABSTRACT. For a wide class of 2D periodic elliptic operators, we show that the global extrema of all spectral band functions are isolated.

Keywords: periodic Schrödinger operator, Bloch eigenvalues, spectral band edges, effective mass.

1. INTRODUCTION

The structure of band edges of periodic Schrödinger operators is an interesting and wide open question of mathematical physics. For example, suppose that a band function $k \mapsto E(k)$ has a minimum (or maximum) k_0 . In solid state physics, the *tensor of effective masses* M_{eff} at k_0 is defined as

$$(1.1) \quad \{M_{\text{eff}}^{-1}\}_{ij} = \pm \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \Big|_{k=k_0}$$

(see [1, Chapter 12, (12.29)] for more details). The choice of the sign depends on whether the extremum is a minimum (“+”, the effective mass of an electron) or a maximum (“−”, the effective mass of a hole). This definition of M_{eff} makes sense only if the right hand side is invertible, i. e. if the critical point k_0 is non-degenerate. This is always true in one dimension, see, for example, [17, Chapter 16]. It is commonly believed that, for $d \geq 2$, the spectral gap edges are non-degenerate for “generic” potentials, see, for example, [15, Conjecture 5.1]. However, there are very few rigorous results in this direction. In [10], it is shown that the lowest eigenvalue for the periodic Schrödinger operator is non-degenerate. The same holds for the two-dimensional Pauli operator, see [4]. A wide class of operators for which the lower edge of the spectrum can be extensively analysed is described in [6]. See also the survey [12] on photonic crystals, where additional references are given. For periodic *magnetic* Schrödinger operators, even the lowest eigenvalue may be degenerate (i. e. the right hand side of (1.1) may vanish, see [19]). Note, however, that this can happen only for sufficiently large magnetic potentials, as shown in [20].

Much less is known about the edges of other bands. In [11], it is established that, for periodic operators of the form $-\Delta + V$ with generic V , the edge of each spectral gap is an extremum of only one band function, but the question of non-degeneracy of these extrema remains open. In [21], it is shown in 2D that for any N there exists a C^∞ -neighbourhood of 0 such that, for potentials V from a dense G_δ -subset of that neighbourhood, the first N band functions are Morse functions. In other words, any finite number of bands is non-degenerate for generic C^∞ -small potentials.

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In the present paper, we establish the following result (Theorem 2.1): for a wide class of 2D periodic elliptic second order operators, any global minimal or maximal value of any band function can only be attained at a discrete set of points. In other words, *the global extrema of each band function are isolated*. In particular, this implies that the level sets corresponding to spectral band edges cannot contain 1D curves. We do not need any genericity or smallness assumptions, and our result holds for all bands, not necessarily for the edges of the spectrum. We formulate the results for “smooth” second order elliptic operators (2.1). We believe that, using methods from [18], the result can be extended to the same generality in which the absolute continuity of the spectrum in 2D is established. The extension beyond dimension 2, however, seems significantly more challenging, as our technique relies heavily on 2D specifics.

An immediate consequence of our result is that Liouville theorems (in the sense of [14, 15]) hold for the operator (2.1) at all gap edges, see Corollary 2.2. Our result can also be used in studying Green’s function asymptotics near spectral gap edges, see [9, 16].

Surprisingly, the statement of the main theorem *fails for discrete periodic Schrödinger operators on \mathbb{Z}^2* , already in the case of a diatomic lattice. We explain the corresponding example of non-isolated extrema in Section 7.

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2. MAIN RESULT

Let

$$\Gamma = \{n_1 b_1 + n_2 b_2, n_1, n_2 \in \mathbb{Z}\}$$

be a lattice in \mathbb{R}^2 , and let Ω be the elementary cell of Γ identified with \mathbb{R}^2/Γ . We will use notation such as $C_{\text{per}}^1(\Omega)$, $H_{\text{per}}^1(\Omega)$ for the classes of functions satisfying periodic boundary conditions.

The periodic magnetic Schrödinger operator with metric g is defined by the expression

$$(2.1) \quad (Hu)(x) = (-i\nabla - A(x))^* g(x) (-i\nabla - A(x))u(x) + V(x)u(x),$$

where the electric potential $V: \mathbb{R}^2 \rightarrow \mathbb{R}$ is Γ -periodic, i.e. assumed to satisfy

$$(2.2) \quad V(x + b_j) = V(x), \quad j = 1, 2, \quad V \in L^\infty(\Omega),$$

and the magnetic potential $A: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is also Γ -periodic and

$$(2.3) \quad A \in C_{\text{per}}^1(\Omega; \mathbb{R}^2), \quad \operatorname{div} A = 0, \quad \int_{\Omega} A(x) dx = 0.$$

Note that the last two conditions can be imposed without loss of generality, see Remark 2.3. The metric g is a Γ -periodic symmetric (2×2) -matrix function satisfying

$$(2.4) \quad g \in C_{\text{per}}^2(\Omega; M_2(\mathbb{R})), \quad g(x) \geq m_g \mathbf{1} > 0, \quad \text{where } \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

for some positive constant m_g . The operator (2.1) is a self-adjoint operator on $L^2(\mathbb{R}^2)$ with the domain being the Sobolev space $H^2(\mathbb{R}^2)$. From the standard Floquet–Bloch theory (see, for example, [17, Chapter 16]), it follows that H is unitarily equivalent to the direct integral

$$(2.5) \quad \int_{\tilde{\Omega}}^{\oplus} H(k) dk,$$

where $\tilde{\Omega}$ is the elementary cell \mathbb{R}^d/Γ' of the dual lattice

$$(2.6) \quad \Gamma' = \{m_1 b'_1 + m_2 b'_2, m_1, m_2 \in 2\pi\mathbb{Z}\}, \quad \langle b_i, b'_j \rangle = \delta_{ij},$$

and the (m -sectorial) operators $H(k)$ in $L^2(\Omega)$ are defined on the domain $H^2_{\text{per}}(\Omega)$ by

$$(2.7) \quad H(k) = (-i\nabla + \bar{k} - A)^* g(-i\nabla + k - A) + V, \quad k \in \mathbb{C}^2.$$

The family (2.7) is an analytic type A operator family with a compact resolvent, in the sense of [8]. This means that the domains $\text{Dom } H(k)$ do not depend on k , and $H(k)u$ is a (weakly) analytic vector-valued function of k_1 and k_2 for any $u \in \text{Dom } H(k) = H^2_{\text{per}}(\Omega)$. Note that, while (2.5) and the statement of the main result only use real values of k , we will often need to consider (2.7) for $k \in \mathbb{C}^2$, and we need \bar{k} in the definition to keep the expression analytic.

For $k \in \mathbb{R}^2$, let us denote the eigenvalues of $H(k)$, taken in the increasing order, by $\lambda_j(k)$. These eigenvalues, considered as functions of k , are called *band functions*. These functions are Γ' -periodic and piecewise real analytic on \mathbb{R}^2 . The spectrum of H

$$\sigma(H) = \bigcup_j [\lambda_j^-, \lambda_j^+]$$

is the union of the *spectral bands* $[\lambda_j^-, \lambda_j^+]$ which are the ranges of $\lambda_j(\cdot)$. It is well known (under much wider assumptions than ours, see [2, 18]) that there are no degenerate bands, i. e. we always have $\lambda_j^- < \lambda_j^+$. The bands, however, can overlap. Our main result concerns the structure of the extrema of band functions.

Theorem 2.1. *Let H be the operator (2.1) with the potentials and the metric satisfying (2.2), (2.3), (2.4). Let λ_* be a global minimal or maximal value of $\lambda_j(\cdot)$. Then the level set*

$$\{k \in \tilde{\Omega} : \lambda_j(k) = \lambda_*\}$$

is finite.

The following Liouville theorem at the edge of the spectrum follows immediately from Theorem 2.1, see [14, Theorem 23 and Remark 6.1] or [15, Theorem 4.4].

Corollary 2.2. *Let H be the operator (2.1) with the potentials and the metric satisfying (2.2), (2.3), (2.4). Then for any $\lambda_* \in \partial(\sigma(H))$, the space of all polynomially bounded solutions of the equation*

$$(-i\nabla - A(x))^* g(x)(-i\nabla - A(x))u(x) + V(x)u(x) = \lambda_* u(x)$$

is finite dimensional.

Remark 2.3. The second and third conditions from (2.3) can be imposed without loss of generality using a gauge transformation $A \mapsto A - \nabla\Phi - |\Omega|^{-1} \int_{\Omega} A(x) dx$ (see, for example, [3, Section 1.2]) with Φ periodic. The addition of $-\nabla\Phi$ is a unitary equivalence transformation of $H(k)$ for all k , and the addition of the last term is equivalent to the change of the quasimomentum $k \mapsto k - |\Omega|^{-1} \int_{\Omega} A(x) dx$. Neither of these changes affects the main result.

The structure of the paper. In Sections 3 – 5, we deal with the case of the *scalar metric* $g(x) = \omega^2(x)\mathbf{1}$. The proof is based on an identity from [7]. This identity shows that the values of k_1 such that $\lambda(k_1e_1 + k_2e_2) = \lambda$, are eigenvalues of a certain non-selfadjoint operator $T_1(k_2, \lambda)$ (see Proposition 3.1 below). Our main observation is that the band edges correspond to *degenerate* eigenvalues of that operator. In Section 3, we introduce the operator T_1 and formulate the main technical result (Theorem 3.3), which shows that the set of the values of k_2 for which $T_1(k_2, \lambda)$ may have degenerate eigenvalues, is discrete. Theorem 3.3 immediately implies the main result. In Section 4, we show that the condition of the operator $T_1(k_2, \lambda)$ having degenerate eigenvalues is an analytic type condition. Hence, either the set of “degenerate” k_2 is discrete, or the operator $T_1(k_2, \lambda)$ has degenerate eigenvalues for all $k_2 \in \mathbb{C}$. In Section 5, we show that the latter case is impossible for the free operator and hence, using perturbation theory and estimates on the symbol, for the perturbed operator. Section 6 describes the reduction of the case of a general C^2 -metric to the case of a scalar one. In Section 7, we give an example of a *discrete* periodic Schrödinger operator for which the statement of the main theorem fails.

3. THE OPERATOR $T_1(k_2, \lambda)$

In this section, we deal with the operator family

$$(3.1) \quad H(k) = (-i\nabla + \bar{k} - A)^* \omega^2 (-i\nabla + k - A) + V,$$

which is a particular case of (2.7); here ω is a scalar function satisfying

$$(3.2) \quad \omega \in C_{\text{per}}^2(\Omega), \quad \omega^2 \geq m_g > 0.$$

Let e_1, e_2 be a standard basis in \mathbb{R}^2 . We also denote the coordinates of k by k_1, k_2 , that is, $k = k_1e_1 + k_2e_2$, and we will often denote $H(k) = H(k_1e_1 + k_2e_2)$ by $H(k_1, k_2)$. Since the statement of the main result is invariant under rotations and dilations of \mathbb{R}^2 , we can fix the following choice of basis of the dual lattice:

$$(3.3) \quad b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2, \quad \text{where } \alpha, \beta \in \mathbb{R}.$$

In the Hilbert space $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$, consider the following unbounded nonselfadjoint operator family:

$$(3.4) \quad T_1(k_2, \lambda) := \begin{pmatrix} 0 & \omega^{-2}I \\ -(H(0, k_2) - \lambda) & 2(i\partial_1 + A_1) - 2i\omega^{-1}\partial_1\omega \end{pmatrix}, \quad k_2, \lambda \in \mathbb{C},$$

where $\text{Dom}(T_1(k_2, \lambda)) = H_{\text{per}}^2(\Omega) \oplus H_{\text{per}}^1(\Omega)$, and $\partial_1 = \frac{\partial}{\partial x_1}$.

The operator $T_1(k_2, \lambda)$ is introduced in order to “linearize” the equation $H(k_1, k_2)u = \lambda u$, considered as a quadratic eigenvalue problem in k_1 , similarly to [7, Lemma 3]. We summarize the properties of the family T_1 (most of which were also used in [7]) in the following proposition.

Proposition 3.1. *The operators $T_1(k_2, \lambda)$ satisfy the following properties.*

- (i) *For all $k_2, \lambda \in \mathbb{C}$, the operator $T_1(k_2, \lambda)$ is closed on the domain $H_{\text{per}}^2(\Omega) \oplus H_{\text{per}}^1(\Omega)$. As a consequence, the family $T_1(\cdot, \lambda)$ is an analytic type A operator family.*
- (ii) *Suppose that $\lambda \notin \sigma(H(k_1, k_2))$. Then $k_1 \notin \sigma(T_1(k_2, \lambda))$, and the resolvent*

$$(3.5) \quad \left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \right)^{-1}$$

is compact in $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$.

- (iii) *$k_1 \in \sigma(T_1(k_2, \lambda))$ if and only if $\lambda \in \sigma(H(k))$, where $k = k_1e_1 + k_2e_2$.*
- (iv) *For all $k_2, \lambda \in \mathbb{C}$, the set $\sigma(T_1(k_2, \lambda))$ is discrete in \mathbb{C} and $2\pi\alpha$ -periodic, where α is defined in (3.3).*

Proof. Part (i). Clearly, the operator $T_1(k_2, \lambda)$ is bounded as an operator from $H_{\text{per}}^2(\Omega) \oplus H_{\text{per}}^1(\Omega)$ to $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$. We also have

$$\left\| T_1(k_2, \lambda) \begin{pmatrix} u \\ v \end{pmatrix} \right\|_{H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)}^2 = \|\omega^{-2}v\|_{H_{\text{per}}^1(\Omega)}^2 + \|-(H(0, k_2) - \lambda)u + (2(i\partial_1 + A_1) - 2i\omega^{-1}\partial_1\omega)v\|_{L^2(\Omega)}^2,$$

from which it follows that the convergence in $T_1(k_2, \lambda)$ -norm implies convergence of v in H^1 and convergence of u in H^2 , so that $T_1(k_2, \lambda)$ is closed on its domain. Strong analyticity in k_2 and λ follows directly from the definition.

Part (ii). Suppose that $\lambda \notin \sigma(H(k))$. Then the equation

$$\left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \right) \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

has a unique solution $\begin{pmatrix} u \\ v \end{pmatrix}$ given by

$$(3.6) \quad \begin{aligned} u &= (H(k) - \lambda)^{-1} \{ (2i\partial_1 + 2A_1 - 2i\omega^{-1}\partial_1\omega - k_1)\omega^2 f - g \}, \\ v &= \omega^2(f + k_1 u). \end{aligned}$$

Let $R(k, \lambda) = (H(k) - \lambda)^{-1}$. By plugging the expression for u into the second equation of (3.6), we can rewrite (3.6) in the operator form, applied to a vector $\begin{pmatrix} f \\ g \end{pmatrix} \in H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$:

$$\begin{aligned} \left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \right)^{-1} \begin{pmatrix} f \\ g \end{pmatrix} &= \begin{pmatrix} 0 & 0 \\ \omega^2 I & 0 \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} + \\ &+ \begin{pmatrix} I & 0 \\ 0 & k_1 \omega^2 \end{pmatrix} R(k, \lambda) \begin{pmatrix} (2i\partial_1 + 2A_1(x) - k_1 - 2i\omega^{-1}(\partial_1\omega)) & -I \\ (2i\partial_1 + 2A_1(x) - k_1 - 2i\omega^{-1}(\partial_1\omega)) & -I \end{pmatrix} \begin{pmatrix} \omega^2 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}. \end{aligned}$$

The first operator in the right hand side is compact in $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$, because the embedding $H_{\text{per}}^1(\Omega) \subset L^2(\Omega)$ is compact. The operator in the second term is compact since $R(k, \lambda)$ is bounded as an operator from $L^2(\Omega)$ to $H_{\text{per}}^2(\Omega)$ and hence is compact from $L^2(\Omega)$ to $H_{\text{per}}^1(\Omega)$. Hence, *the resolvent of $T_1(k_2, \lambda)$ is compact*, which completes the proof of Part (ii).

Part (iii). The “only if” part is included in Part (ii). To establish “if” part, suppose that $H(k)u = \lambda u$. Then $u \in H_{\text{per}}^2(\Omega)$, and

$$T_1(k_2, \lambda) \begin{pmatrix} u \\ k_1 \omega^2 u \end{pmatrix} = k_1 \begin{pmatrix} u \\ k_1 \omega^2 u \end{pmatrix}.$$

This completes the proof of (iii).

Part (iv). From the proofs of the absolute continuity of the spectrum (see e.g., [2]), it follows that, for any $\lambda, k_2 \in \mathbb{C}$, the set $\{k_1 : \lambda \in \sigma(H(k_1, k_2))\}$ is discrete. Hence, there exists at least one value of k_1 such that the resolvent (3.5) exists, which, together with Part (ii), implies that $\sigma(T(k_2, \lambda))$ is discrete. Periodicity of the spectrum follows from the fact that $H(k)$ is unitarily equivalent to $H(k + b')$ for any $b' \in \Gamma'$ (see (2.6)), and so $H(k_1, k_2)$ is unitarily equivalent to $H(k_1 + 2\pi\alpha, k_2)$. ■

In the sequel, by “the multiplicity of an isolated eigenvalue” we will mean *algebraic multiplicity*, i.e. the dimension of the range of the corresponding Riesz projection. We will call an eigenvalue *degenerate* if its algebraic multiplicity is greater than or equal to 2. Otherwise, an eigenvalue is called *simple*.

Lemma 3.2. *Suppose that a band function $\lambda_j(\cdot)$ attains its local minimum or maximum value λ_* at $k^* = k_1^*e_1 + k_2^*e_2 \in \mathbb{R}^2$. Then k_1^* is an eigenvalue of $T_1(k_2^*, \lambda_*)$ of the (algebraic) multiplicity at least two.*

Proof. By Proposition 3.1 k_1^* is an eigenvalue of $T_1(k_2^*, \lambda_*)$. For some $\varepsilon > 0$, there are no other eigenvalues of $T_1(k_2^*, \lambda_*)$ within the closed disc $\overline{B_\varepsilon(k_1^*)}$. Let

$$P(k_2^*, \lambda) := -\frac{1}{2\pi i} \oint_{\partial B_\varepsilon(k_1^*)} (T_1(k_2, \lambda) - \varkappa I)^{-1} d\varkappa$$

be the Riesz projection. The standard arguments [8, Section IV.3.5] show that, for some $\delta > 0$, $\text{rank } P(k_2^*, \lambda)$ is continuous in λ as long as $|\lambda - \lambda_*| < \delta$. Without loss of generality, assume that k^* is a local minimum of $\lambda_j(\cdot)$.

From the proofs of the absolute continuity of the spectrum (see e.g., [2]), it follows that $\lambda_j(k)$ cannot be constant in k_1 on any interval. Then, for a sufficiently small $\delta > 0$, the equation $\lambda_j(k_1, k_2^*) = \lambda_* + \delta$ has at least two different solutions as an equation in k_1 (note that these arguments do not use any analyticity of $\lambda_j(\cdot, k_2^*)$, only continuity). Hence, by Part (iii) of Proposition 3.1, $\text{rank } P(k_2^*, \lambda_* + \delta) \geq 2$ for all sufficiently small δ , and therefore $\text{rank } P(k_2^*, \lambda_*) \geq 2$ due to continuity. ■

The following is the main technical result of the paper.

Theorem 3.3. *Suppose that the coefficients ω, A, V satisfy (3.2), (2.3), (2.2). For any $\lambda \in \mathbb{R}$, the set*

$$\{k_2 \in \mathbb{R} : \text{the operator } T_1(k_2, \lambda) \text{ has at least one real degenerate eigenvalue}\}$$

is discrete.

Proof of Theorem 2.1: the case of a scalar metric. Fix a band function $\lambda_j(\cdot)$ and assume that λ_* is a minimum or a maximum of λ_j . From Theorem 3.3 and Lemma 3.2, the set of possible k_2 such that for some k_1 we have $\lambda_j(k) = \lambda_*$, is discrete. For each of these k_2 , the set of possible values of k_1 is also discrete by Proposition 3.1. ■

Theorem 3.3 is proved in Sections 4 and 5. The rest of the proof of Theorem 2.1 is a (mostly standard) argument of transforming a general metric to a scalar metric by introducing isothermal coordinates. This is done in Section 6.

4. PROOF OF THEOREM 3.3

Let

$$p(z) = z^n + a_{n-1}z^{n-1} + \dots + a_0$$

be a monic polynomial with roots z_1, \dots, z_n . The *discriminant* of p is defined as

$$\Delta(p) = \prod_{1 \leq i < j \leq n} (z_i - z_j)^2.$$

It is clear that $\Delta(p)$ vanishes if and only if p has roots of multiplicity greater than or equal to 2. It is well known (see, for example, [22, Section 5.9]) that $\Delta(p)$ is a polynomial function of the coefficients a_0, \dots, a_{n-1} . The following fact is probably known, but we could not find it in the literature.

Lemma 4.1. *Let \mathcal{C} be a simple closed piecewise smooth contour in \mathbb{C} , and let $\{T(z), z \in \mathcal{D}\}$ be an operator family of type A in a Hilbert space \mathcal{H} analytic in a simply connected domain*

$\mathcal{D} \subset \mathbb{C}$. Suppose that, for all $z \in \mathcal{D}$, the spectrum of $T(z)$ in the interior of \mathcal{C} is discrete and finite, and $\sigma(T(z)) \cap \mathcal{C} = \emptyset$. Then the set

$$\{z \in \mathcal{D} : T(z) \text{ has at least one degenerate eigenvalue in the interior of } \mathcal{C}\}$$

is a null-set of a function analytic in \mathcal{D} , and hence this set either coincides with \mathcal{D} or is discrete in \mathcal{D} .

Proof. Let

$$P(z) := -\frac{1}{2\pi i} \oint_{\mathcal{C}} (T(z) - \kappa I)^{-1} d\kappa$$

be the Riesz projection. By assumption, $n := \text{rank } P(z) = \text{const}$ is finite and independent on z , and $P(z)$ is analytic in \mathcal{D} . Fix $z_0 \in \mathcal{D}$. The results of [8, Section VII.1.3] imply that there exists an analytic in \mathcal{D} bounded operator-valued function $U : \mathcal{D} \rightarrow \mathcal{B}(\mathcal{H})^1$ such that $U(\cdot)^{-1}$ is also analytic in \mathcal{D} and $P(z) = U(z)P(z_0)U(z)^{-1}$. Take

$$T_0(z) := U(z)^{-1}T(z)U(z)|_{\text{ran } P(z_0)}.$$

The family $T_0(z)$ is an analytic operator family acting in a fixed finite-dimensional space that has the same eigenvalues and multiplicities as $T(z)$ restricted to $\text{ran } P(z)$. The monic polynomial $p_z(\kappa) = (-1)^n \det(T_0(z) - \kappa)$ is the characteristic polynomial of $T_0(z)$ and has the coefficients analytic in \mathcal{D} (in the variable z). Hence, its discriminant $\Delta(p_z)$ is also an analytic function in \mathcal{D} vanishing if and only if $T_0(z)$ (and, as a consequence, $T(z)$) has degenerate eigenvalues in the interior of \mathcal{C} . ■

Recall that we had a special choice of basis in Γ' ,

$$b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2.$$

Let also

$$k = k_1 e_1 + k_2 e_2, \quad k_1 = r_1 + il_1, \quad k_2 = r_2 + il_2.$$

The following two theorems are the main technical statements of the paper. We postpone the proofs to the next section.

Without loss of generality, one can assume $\lambda = 0$ by choosing a different V . In the sequel, we will make this assumption and drop λ from the notation for T_1 , that is, $T_1(k_2) := T_1(k_2, 0)$.

Theorem 4.2. *Let $\delta > 0$. There exist $C = C(A, V, \omega)$ and $C_1 = C_1(A, V, \omega, \delta) \in 2\pi\mathbb{Z}$ such that operator $H(k)$ defined in (3.1) is invertible and satisfies*

$$\|H(k)^{-1}\| \leq \frac{C}{|l_1|\delta^2}$$

provided that $\text{dist}(r_2, 2\pi\mathbb{Z}) \geq \delta$, $l_1 \in 2\pi\mathbb{Z}$, $|l_1| \geq C_1$. As a consequence, the horizontal lines $\text{Im } k_1 = \pm C_1$ have empty intersection with $\sigma(T_1(k_2))$.

Theorem 4.3. *There exists $l = l(A, V, \omega) \in 2\pi\mathbb{Z}$ such that, for all $n \in 2\pi\mathbb{Z}$, the spectrum of $T_1(k_2)$ is simple for $k_2 = \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$.*

Proof of Theorem 3.3. Assume the contrary, i. e. that the set of $k_2 \in \mathbb{R}$ for which $T_1(k_2)$ has real degenerate eigenvalues has a limit point $k_2^{(0)}$ (as above we assume $\lambda = 0$). Let us consider two cases.

Case 1. Suppose that $\text{dist}(k_2^{(0)}, 2\pi\mathbb{Z}) > 0$. Take $\delta = \min\{\pi/2, \text{dist}(k_2^{(0)}, 2\pi\mathbb{Z})\}$. There exists a single $n \in 2\pi\mathbb{Z}$ such that $k_2^{(0)} \in [n + \delta, n + 2\pi - \delta]$. Let \mathcal{C}_0 be a path in the k_2 -plane starting at

¹ $\mathcal{B}(\mathcal{H})$ denotes the algebra of bounded operators on a Hilbert space H .

$k_2^{(0)}$, then going straight towards the point $\frac{\pi}{2} + n$, and then going vertically towards the point $k_2^{(1)} := \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$ from Theorem 4.3.

The points $k_2 \in \mathcal{C}_0$ satisfy the assumptions of Theorem 4.2. Let us consider the eigenvalues of $T_1(k_2)$ lying within the strip $|\operatorname{Im} k_1| < C_1$, where C_1 is the constant from Theorem 4.2. They form a discrete $2\pi\alpha$ -periodic set. For each $k_2 \in \mathcal{C}_0$ there exists a point $r(k_2) \in \mathbb{R}$ which is *not* a real part of any of these eigenvalues. Moreover, by continuity arguments, this also holds in a small (complex) neighbourhood of k_2 . Let us cover \mathcal{C}_0 by a finite number of these neighbourhoods \mathcal{D}_j , $j = 1, \dots, p$, so that $k_2^{(0)} \in \mathcal{D}_1$ and $k_2^{(1)} \in \mathcal{D}_p$ and denote the corresponding values of $r(k_2)$ by r_j . For each j , denote by \mathcal{C}_j the boundary of the following rectangle:

$$r_j < \operatorname{Re} k_1 < r_j + 2\pi\alpha, \quad -C_1 < \operatorname{Im} k_1 < C_1.$$

Informally speaking, each rectangle contains all eigenvalues that we are interested in: they are initially on the real line, they cannot cross the lines $\operatorname{Im} k_1 = \pm C_1$, and the pictures to the right and to the left copy the picture in the rectangle due to periodicity.

Let us apply Lemma 4.1 to each of the domains \mathcal{D}_j and contours \mathcal{C}_j . Due to Theorem 4.3, the spectrum of $T_1(k_2^{(1)})$ is simple, and hence the set of “degenerate” k_2 should be discrete in a neighbourhood \mathcal{D}_p of $k_2^{(1)}$. By the standard arguments of analytic continuation, it should also be discrete in every neighbourhood $\mathcal{D}_1, \dots, \mathcal{D}_p$. However, since $k_2^{(0)} \in \mathcal{D}_1$, it is not discrete in \mathcal{D}_1 , which is a contradiction.

Case 2. Suppose that $k_2^{(0)} \in 2\pi\mathbb{Z}$. The set of *real* eigenvalues of $T_1(k_2^{(0)})$ is, again, discrete and $2\pi\alpha$ -periodic. Let us surround the eigenvalues on one period by a contour \mathcal{C} not containing any other eigenvalues. In a small neighbourhood \mathcal{D}_0 of $k_2^{(0)}$, these eigenvalues still stay within \mathcal{C} . Apply Lemma 4.1 to \mathcal{C} and \mathcal{D}_0 . Again, since the set of “degenerate” values of k_2 is not discrete in \mathcal{D}_0 , it should coincide with \mathcal{D}_0 , and hence there exists at least one more point with the same property that belongs to $\mathbb{R} \setminus 2\pi\mathbb{Z}$, and thus the situation reduces to Case 1. ■

5. PROOFS OF THEOREMS 4.2, 4.3

Let us start by recalling some notation introduced above,

$$b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2, \quad \alpha, \beta \in \mathbb{R};$$

$$k = k_1 e_1 + k_2 e_2, \quad k_1 = r_1 + i l_1, \quad k_2 = r_2 + i l_2, \quad r_1, r_2, l_1, l_2 \in \mathbb{R}.$$

In this section, we will emphasize the dependence of H on g, A, V and use the notation $H(k; g, A, V)$. Consider the free operator $H_0(k) := H(k; \mathbf{1}, 0, 0)$. Its eigenfunctions are of the form

$$\exp\{im \cdot x\} = \exp\{i(m_1 b'_1 + m_2 b'_2) \cdot (x_1 e_1 + x_2 e_2)\} = \exp\{i((\alpha m_1 + \beta m_2)x_1 + m_2 x_2)\},$$

$$m = m_1 b'_1 + m_2 b'_2 \in \Gamma', \quad m_1, m_2 \in 2\pi\mathbb{Z},$$

and

$$H_0(k) \exp\{im \cdot x\} = ((-i\partial_1 + k_1)^2 + (-i\partial_2 + k_2)^2) \exp\{im \cdot x\} = h_m(k) \exp\{im \cdot x\},$$

where $h_m(k)$ is the symbol of $H_0(k)$:

$$h_m(k) = (\alpha m_1 + \beta m_2 + k_1)^2 + (m_2 + k_2)^2 = q_m^+(k) q_m^-(k),$$

$$q_m^\pm(k) = \alpha m_1 + \beta m_2 + r_1 \mp l_2 + i(l_1 \pm m_2 \pm r_2).$$

Let also $Q^\pm(k)$ be the operators with symbols $q_m^\pm(k)$ respectively, so that $H_0(k) = Q^+(k)Q^-(k)$. Suppose that the magnetic potential A satisfies (2.3). Then there exists a Γ -periodic scalar function $\varphi \in C_{\text{per}}^2(\Omega)$ such that

$$(5.1) \quad (\nabla\varphi)(x) = A_2(x)e_1 - A_1(x)e_2, \quad \int_{\Omega} \varphi(x) dx = 0, \quad \|\varphi\|_{C^2(\Omega)} \leq C\|A\|_{C^1(\Omega)}.$$

Let also

$$B(x) = \partial_1 A_2(x) - \partial_2 A_1(x), \quad w(x) := e^{-2\varphi(x)}.$$

The operator $H(k; \mathbf{1}, A, B)$ is called *the Pauli operator* (more precisely, a block of the Pauli operator). The following is proved in [2] and allows us to reduce the case of the magnetic potential, essentially, to the case of the free operator.

Proposition 5.1. *Under the above assumptions, if $Q^\pm(k)$ are invertible, then $H(k; \mathbf{1}, A, B)$ is also invertible, and*

$$(5.2) \quad H(k; \mathbf{1}, A, B)^{-1} = e^\varphi Q^-(k)^{-1} e^{-2\varphi} Q^+(k)^{-1} e^\varphi = \\ = e^{\varphi(x)} H_0(k)^{-1} \{e^{-\varphi} + (-i\partial_1 w + \partial_2 w) Q^+(k)^{-1} e^\varphi\}.$$

The following proposition can also be easily verified, see [5]. It will be used to reduce the case of a scalar metric $g = \omega^2 \mathbf{1}$ to the case $g = \mathbf{1}$.

Proposition 5.2. *Suppose that $\omega \in C_{\text{per}}^2(\Omega)$, $V \in L^\infty(\Omega)$, $A \in C_{\text{per}}^1(\Omega)$. Then*

$$(5.3) \quad H(k; \omega^2 \mathbf{1}, A, V) = \omega H(k; \mathbf{1}, A, \omega^{-2} V + \omega^{-1} \Delta \omega) \omega,$$

$$(5.4) \quad \omega H(k; \mathbf{1}, A, V) \omega = H(k; \omega^2 \mathbf{1}, A, \omega^2 V - \omega \Delta \omega).$$

Proof of Theorem 4.2. Suppose that $\text{dist}(r_2, 2\pi\mathbb{Z}) = \delta$. Since $l_1 \pm m_2 \in 2\pi\mathbb{Z}$, we have $|q_m^\pm(k)| \geq \delta$. In addition, $\text{Im } q_m^+(k) + \text{Im } q_m^-(k) = 2l_1$, and hence we either have $|q_m^+(k)| \geq |l_1|$ or $|q_m^-(k)| \geq |l_1|$. Combining these estimates, we obtain $|h_m(k)| \geq |l_1|\delta$, and

$$(5.5) \quad \|H_0(k)^{-1}\| \leq \frac{1}{|l_1|\delta}, \quad \|Q^+(k)^{-1}\| \leq \frac{1}{\delta},$$

which completes the proof for $A = 0$, $V = 0$, $\omega = 1$. If $A \neq 0$ and $V(x) = B(x)$, then, from (5.2) and (5.5), we get

$$(5.6) \quad \|H(k; \mathbf{1}, A, B)^{-1}\| \leq \frac{C}{|l_1|\delta^2},$$

where C depends on A via w and φ . The standard Neumann series arguments imply that the bound (5.6) holds for the operator $H(k, \mathbf{1}, A, V)$ with arbitrary $V \in L^\infty(\Omega)$ (and maybe a different C) for sufficiently large l_1 , say,

$$|l_1| \geq \frac{2\|V - B\|_{L^\infty(\Omega)} C}{\delta^2}.$$

The case of arbitrary ω follows from Proposition 5.2. ■

We now make some preparations for the proof of Theorem 4.3. Fix k_2 as in the formulation of the theorem, so that

$$(5.7) \quad r_2 = \frac{\pi}{2} + n, \quad l_2 = \left(\frac{\pi}{2} + l\right) \alpha, \quad l, n \in 2\pi\mathbb{Z}.$$

For these k_2 , define

$$\Sigma_n := \{k_1 \in \mathbb{C} : h_m(k_1, k_2) = 0 \text{ for some } m_1, m_2 \in 2\pi\mathbb{Z}\}.$$

In other words, it is the set of k_1 for which $H_0(k_1, k_2)$ is not invertible. A simple computation shows that Σ_n consists of points $r_1 + il_1$ of the following form:

$$(5.8) \quad \begin{cases} r_1 = -\alpha m_1 - \beta m_2 \mp \left(\frac{\pi}{2} + l\right) \alpha \\ l_1 = \pm \left(\frac{\pi}{2} + n + m_2\right) \end{cases}, \quad m_1, m_2 \in 2\pi\mathbb{Z}.$$

Since one can replace the variables m_1 by $m_1 + l$, one can see that *the set Σ_n does not depend on l .*

Let us describe the set Σ_n in more detail. First of all, it is easy to see that different values of (m_1, m_2) give different points of Σ_n , as m_2 and the signs are uniquely determined by the value of l_1 , and m_1 is determined by r_1 afterwards. Next, the set Σ_n lies on the union of horizontal lines $\text{Im } k_1 \in \pi/2 + \pi\mathbb{Z}$. On each line, it is a sequence of equally spaced points with the spacings $2\pi\alpha$.

We will also need another set G_n defined by

$$G_n := (\mathbb{R} + i\pi\mathbb{Z}) \cup \bigcup_{z \in \Sigma_n} \left(z + \pi\alpha + i \left[-\frac{\pi}{2}, \frac{\pi}{2} \right] \right).$$

The set G_n consists of horizontal lines $\text{Im } k_1 \in \pi\mathbb{Z}$ separating the horizontal lines of Σ_n . In addition, for each point of Σ_n , we include a vertical line segment of the length π separating this point from the next point of Σ_n lying on the same line. One can imagine G_n as a “brick wall” consisting of rectangles such that there is exactly one element of Σ_n inside of each rectangle.

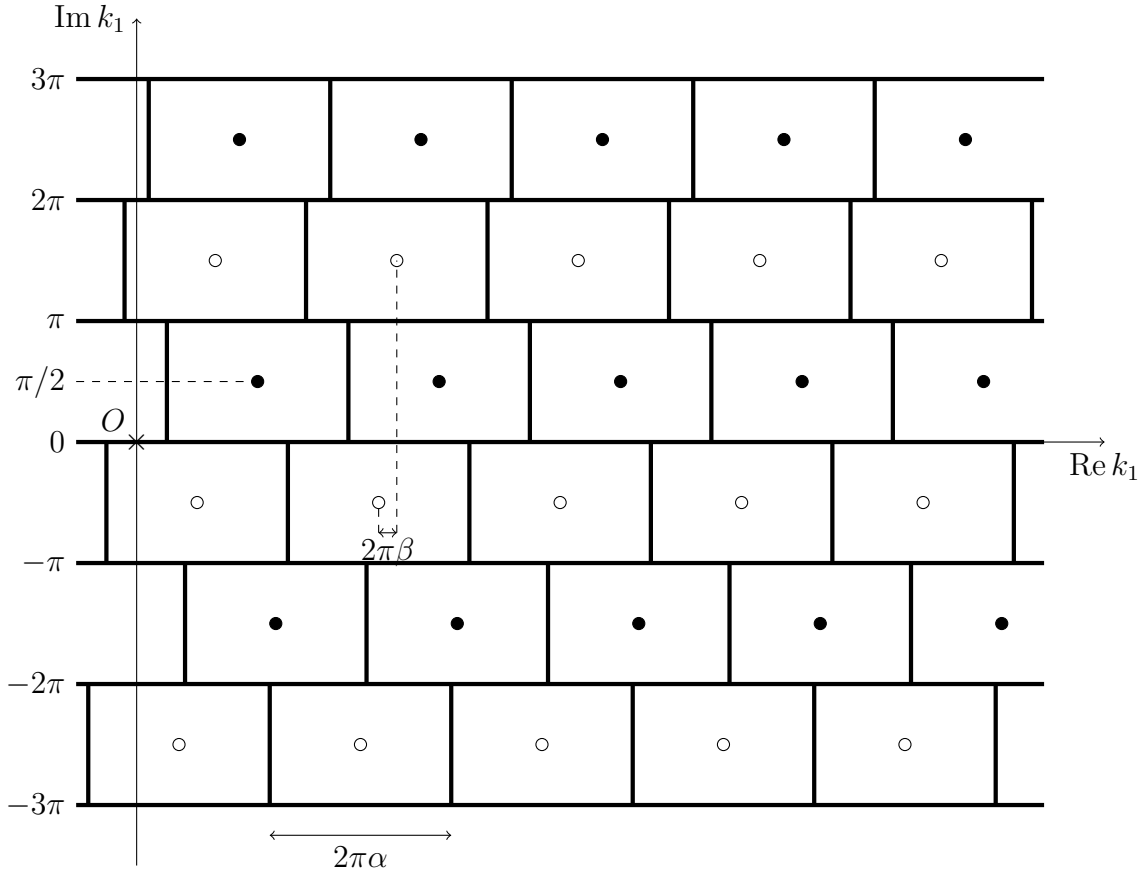


FIGURE 1. The sets Σ_n and G_n .

On Figure 1, an example of Σ_n and G_n is shown for $n = 0$, $\alpha = 0.75$, $\beta = 0.075$. The set G_n is represented by thick lines, and the locations of points of Σ_n are indicated by black and white circles, corresponding to the upper or lower choice of signs in (5.8), respectively.

Lemma 5.3. *Suppose that $k_1 \in G_n$, $k_2 = \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$, where $l, n \in 2\pi\mathbb{Z}$. Then*

$$|h_m(k)| \geq C|l|$$

uniformly in $m_1, m_2 \in 2\pi\mathbb{Z}$.

Proof. Since $|\operatorname{Re} q_m^+(k) - \operatorname{Re} q_m^-(k)| = 2|l_2| \geq C|l|$, we have for each m either $|q_m^+(k)| \geq \frac{1}{2}C|l|$ or $|q_m^-(k)| \geq \frac{1}{2}C|l|$. On the other hand, both $|q_m^+(k)|$ and $|q_m^-(k)|$ are distances from k_1 to a certain point of Σ_n , which is bounded from below by a positive constant,

$$(5.9) \quad |q_m^\pm(k)| \geq \operatorname{dist}(k_1, \Sigma_n) \geq \operatorname{dist}(G_n, \Sigma_n) = \min \left\{ \frac{\pi}{2}, \pi\alpha \right\}.$$

The combination of these estimates completes the proof of the lemma. ■

Remark 5.4. Lemma 5.3 is the main ingredient of the proof that relies on the assumption $d = 2$. In $d \geq 3$, one cannot construct a set G_n with similar properties and constant size of the bricks.

Corollary 5.5. *Under the assumptions of Lemma 5.3, there exists $L_0(A, V, \omega) > 0$ such that, if $|l| > L_0(\omega, A, V)$, then the operator $H(k; \omega^2 \mathbf{1}, A, V)$ is invertible and*

$$\|H(k; \omega^2 \mathbf{1}, A, V)^{-1}\| \leq \frac{C(\omega, A, V)}{|l|},$$

where the constants C and L_0 depend only on $\|A\|_{C^1(\Omega)}$, $\|V\|_{L^\infty(\Omega)}$, $\|\omega\|_{C^2(\Omega)}$ and on the constant m_g from (3.2).

Proof. From Proposition 5.2, we have

$$\|H(k; \omega^2 \mathbf{1}, A, V)^{-1}\| \leq m_g^{-2} \|H(k; \mathbf{1}, A, V_\omega)^{-1}\|,$$

where

$$V_\omega = \omega^{-2}V + \omega^{-1}\Delta\omega$$

and therefore

$$\|V_\omega\|_{L^\infty(\Omega)} \leq m_g^{-2}\|V\|_{L^\infty(\Omega)} + m_g^{-1}\|\omega\|_{C^2(\Omega)}.$$

From (5.2), (5.1), Lemma 5.3, and (5.9), we have

$$\|H(k; \mathbf{1}, A, B)^{-1}\| \leq C(A) \|H_0(k)^{-1}\| \leq \frac{C_1(A)}{|l|},$$

where $C(A)$, $C_1(A)$ depend only on $\|A\|_{C^1(\Omega)}$. Since $\|B\|_{L^\infty(\Omega)} \leq 2\|A\|_{C^1(\Omega)}$, we can use the same Neumann series argument as in the proof of Theorem 4.2 to replace B by V_ω . ■

Proof of Theorem 4.3. Denote by $T_\mu(k_2)$ the operator $T_1(k_2)$ with V , A , ω replaced by μV , μA and $\mu\omega + (1 - \mu)$ respectively. It is a one-parametric family connecting the “free” operator $T_0(k_2)$ with $T_1(k_2)$.

It is easy to see that $\sigma(T_0(k_2)) = \Sigma_n$, because Σ_n is exactly the set of $k_1 \in \mathbb{C}$ for which the symbol of $H_0(k)$ is not invertible. Moreover, an easy computation shows that, for each $k_1 \in \Sigma_n$, the corresponding eigenspace is one-dimensional and is spanned by $\begin{pmatrix} e^{im \cdot x} \\ k_1 e^{im \cdot x} \end{pmatrix}$, where m is determined by k_1 via (5.8). Note that each value of m appears twice (for two different

values of k_1) because of two possible signs. Hence, the total collection of eigenvectors spans $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$, so there are no Jordan cells and *the spectrum of $T_0(k_2)$ is simple*.

It remains to prove that $T_1(k_2)$ also has simple spectrum. Consider the Riesz projection of $T_\mu(k_2)$ with respect to the boundary of some rectangle of G_n . For $\mu = 0$, the rectangle contains exactly one simple eigenvalue, and the range of the projection has dimension 1. Let us increase μ . The only way for the dimension of the range to change is to have an eigenvalue of $T_\mu(k_2)$ approach the set G_n . This, however, is impossible for $\mu \in [0, 1]$ due to Corollary 5.5, and hence the eigenvalues of $T_1(k_2)$ stay simple. ■

Remark 5.6. The proof of Theorem 4.3 is based on the ideas of [7, Section VI].

6. THE CASE OF VARIABLE METRIC

In this section we show how to reduce the case of an operator with arbitrary metric g satisfying (2.4) to the case of the scalar metric. The technical difference with standard arguments such as in [18] is that we need to keep track of the quasimomentum in order to ensure that it is transformed linearly. This is done by an additional “gauge transformation”. The following proposition establishes the existence of *global isometric coordinates* in which the metric g becomes scalar. See [13, Proposition 18] for the proof.

Proposition 6.1. *Suppose that g satisfies (2.4). Then there exists a basis b_1^*, b_2^* of \mathbb{R}^2 and a one-to-one map $\Psi: \mathbb{R}^2 \rightarrow \mathbb{R}^2$, $\Psi \in C^3(\mathbb{R}^2)$, $\det \Psi'(x) \neq 0$,*

$$\Psi(0) = 0, \quad \Psi(x + n_1 b_1 + n_2 b_2) = \Psi(x) + n_1 b_1^* + n_2 b_2^*, \quad \forall n_1, n_2 \in \mathbb{Z},$$

such that

$$(6.1) \quad |\det \Psi'(x)|^{-1} \Psi'(x) g(x) \Psi'(x)^t = \omega^2(\Psi(x)) \mathbf{1},$$

where $\omega \in C^2(\mathbb{R}^2)$ is a strictly positive scalar function periodic with respect to the lattice Γ_ spanned by b_1^* and b_2^* .*

Let us introduce some notation. Suppose that the operator $H(g, A, V)$ satisfies the assumptions of Theorem 2.1. Let Ψ be the transformation obtained from Proposition 6.1. Denote by $T_*: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ the linear transformation defined by $T_*(b_1) = b_1^*$, $T_*(b_2) = b_2^*$. The transformation T_* , as well as the map Ψ , transforms the lattice Γ into Γ_* . Let also

$$y = \Psi(x), \quad A_*(y) = (\Psi'(x)^{-1})^t A(x), \quad V_*(y) = \psi_*(y)^{-2} V(x), \quad \psi_*(y) = |\det \Psi'(x)|^{1/2}.$$

Let also

$$\Omega_\Psi = \Psi(\Omega), \quad \Omega_* = \{y_1 b_1^* + y_2 b_2^*, \quad y_1, y_2 \in [0, 1)\}.$$

Note that both Ω_* and Ω_Ψ are fundamental domains of Γ_* , and there is a natural correspondence between $L^2(\Omega_*)$ and $L^2(\Omega_\Psi)$, as both can be identified with \mathbb{R}^d/Γ_* .

Lemma 6.2. *In the above notation, let $\Phi: L^2(\Omega) \rightarrow L^2(\Omega_*)$ be the unitary operator of change of variables:*

$$u(x) = \psi_*(y)(\Phi u)(y), \quad y = \Psi(x),$$

where u is considered as an element of $L^2(\Omega_)$. Then*

$$\Phi H(0; g, A, V) \Phi^{-1} = \psi_* H(0; \omega^2 \mathbf{1}, A_*, V_*) \psi_*.$$

Proof. Let $v = \Phi u$, and let us extend it Γ_* -periodically into \mathbb{R}^d . Then, due to (6.1) and the change of variable rule, the quadratic form of the left hand side applied to v is equal to

$$(H(0; g, A, V) \Phi^{-1} v, \Phi^{-1} v)_{L^2(\Omega)} = (H(0; g, A, V) u, u)_{L^2(\Omega)} =$$

$$\begin{aligned}
&= \int_{\Omega} \langle g(x)(-i\nabla_x - A(x))u(x), (-i\nabla_x - A(x))u(x) \rangle dx + \int_{\Omega} V(x)|u(x)|^2 dx \\
&= \int_{\Omega_{\Psi}} \langle \omega^2(y)(-i\nabla_y - A_*(y))\psi_*(y)v(y), (-i\nabla_y - A_*(y))\psi_*(y)v(y) \rangle dy + \int_{\Omega_{\Psi}} V_*(y)\psi_*(y)^2|v(y)|^2 dy = \\
&= \int_{\Omega_*} \langle \omega^2(y)(-i\nabla_y - A_*(y))\psi_*(y)v(y), (-i\nabla_y - A_*(y))\psi_*(y)v(y) \rangle dy + \int_{\Omega_*} V_*(y)\psi_*(y)^2|v(y)|^2 dy = \\
&= (H(0; \omega^2 \mathbf{1}, A_*, V_*)\psi_*v, \psi_*v)_{L^2(\Omega_*)}. \blacksquare
\end{aligned}$$

Theorem 6.3. *Suppose that $k \in \mathbb{R}^2$. Under the assumptions of Theorem 2.1, the operator $H(k; g, A, V)$ is unitarily equivalent to the operator*

$$(6.2) \quad H((T_*^{-1})^t k, \omega^2 \psi_*^2 \mathbf{1}, A_*, \psi_*^2 V_* + \psi_*^2 \omega \Delta \omega - \psi_* \omega \Delta (\psi_* \omega))$$

acting in $L^2(\Omega_*)$, where Ω_* is the elementary cell of Γ_* , and $T_*, \omega, \psi_*, A_*, V_*$ are defined above.

Proof. We will perform the required unitary transformation in several steps. First, let us note that $H(k; g, A, V) = H(0; g, A - k, V)$. Consider the unitary transformation $u(x) = e^{i\alpha(x)}v(x)$, where $\alpha \in C_{\text{per}}^1(\Omega)$. Under this transformation, the operator $H(k; g, A, V)$ becomes $H(0; g, A - k - \nabla \alpha, V)$. Take $\alpha(x) = k(T_*^{-1}\Psi(x) - x)$. This function is Γ -periodic, and

$$(\nabla \alpha)(x) = \Psi'(x)^t (T_*^{-1})^t k - k.$$

Hence, the operator $H(k; g, A, V)$ is unitarily equivalent to $H(0, g, A - \Psi'(x)^t (T_*^{-1})^t k, V)$, which, by Lemma 6.2, is equivalent to

$$\psi_* H(0, \omega^2 \mathbf{1}, A_* - (T_*^{-1})^t k, V_*) \psi_* = \psi_* H((T_*^{-1})^t k, \omega^2 \mathbf{1}, A_*, V_*) \psi_*.$$

Applying (5.3) and then (5.4), we ultimately obtain

$$\begin{aligned}
\psi_* H((T_*^{-1})^t k, \omega^2 \mathbf{1}, A_*, V_*) \psi_* &= \omega \psi_* H((T_*^{-1})^t k, \mathbf{1}, A_*, \omega^{-2} V_* + \omega^{-1} \Delta \omega) \omega \psi_* = \\
&= H((T_*^{-1})^t k, \omega^2 \psi_*^2 \mathbf{1}, A_*, \psi_*^2 V_* + \psi_*^2 \omega \Delta \omega - \psi_* \omega \Delta (\psi_* \omega)). \blacksquare
\end{aligned}$$

This completes the proof of Theorem 2.1, because its statement has already been established for the operators (6.2), and the operator families $H(k; g, A, V)$ and (6.2) have the same band functions up to a linear transformation of k .

7. AN EXAMPLE OF DEGENERATE BAND EDGE IN THE DISCRETE CASE

Consider the discrete Schrödinger operator $H = \mathcal{D} + V$ in $l^2(\mathbb{Z}^2)$, where

$$(\mathcal{D}u)_n = \frac{1}{2} (u_{n+e_1} + u_{n-e_1} + u_{n+e_2} + u_{n-e_2}), \quad n \in \mathbb{Z}^2,$$

is the discrete Laplace operator, and V is the operator of multiplication by the potential given by

$$(Vu)_n = \begin{cases} v_0 u_n, & \text{if } (n_1 + n_2) \text{ is even,} \\ v_1 u_n, & \text{if } (n_1 + n_2) \text{ is odd;} \end{cases}$$

the real numbers v_0 and v_1 are fixed. In other words, the lattice is formed by two different types of atoms placed in a chessboard order, and V is periodic with respect to the lattice spanned by $\{2e_1, e_1 + e_2\}$. The corresponding Floquet-Bloch transform

$$F : l^2(\mathbb{Z}^2) \rightarrow L^2(\tilde{\mathcal{O}} \times \{0; 1\})$$

is given by

$$(Fu)(k; m) = \frac{1}{\pi\sqrt{2}} \sum_{n_1+n_2 \equiv m \pmod{2}} e^{-ikn} u_n.$$

Here $k \in \tilde{\mathcal{O}} = \{k \in \mathbb{R}^2 : |k_1 + k_2| < \pi\}$, $m = 0$ or $m = 1$; the operator F is unitary. It is easy to see that

$$FHF^* = \int_{\tilde{\mathcal{O}}}^{\oplus} H(k) dk,$$

where $H(k)$ is a self-adjoint operator in \mathbb{C}^2 ,

$$H(k) = \begin{pmatrix} v_0 & \cos k_1 + \cos k_2 \\ \cos k_1 + \cos k_2 & v_1 \end{pmatrix}.$$

Eigenvalues of this matrix are

$$\lambda_{\pm}(k) = \frac{v_0 + v_1}{2} \pm \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + (\cos k_1 + \cos k_2)^2},$$

from which it follows that

$$\min \lambda_- = \frac{v_0 + v_1}{2} - \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + 4}, \quad \max \lambda_- = \min(v_0, v_1),$$

$$\min \lambda_+ = \max(v_0, v_1), \quad \max \lambda_+ = \frac{v_0 + v_1}{2} + \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + 4}.$$

So, the spectrum of the operator H consists of two bands separated by a gap, whenever $v_0 \neq v_1$.

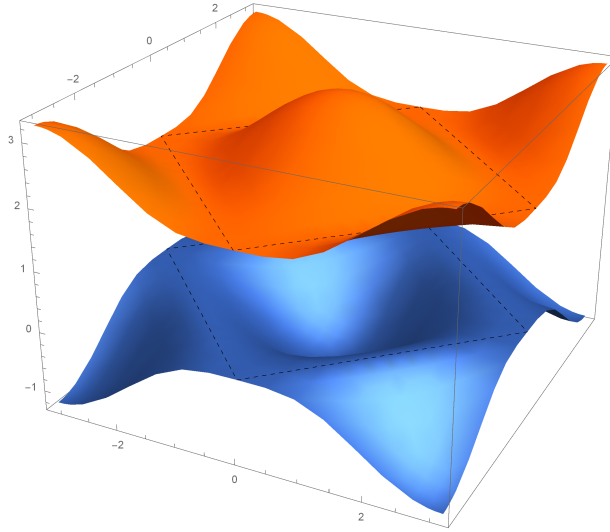


FIGURE 2. The band functions $\lambda_+(k)$ and $\lambda_-(k)$.

The edges of this gap (v_0 and v_1 respectively) are attained on the set

$$\{k \in \mathbb{R}^2 : \cos k_1 + \cos k_2 = 0\} = \{k \in \mathbb{R}^2 : k_1 \pm k_2 = (2p+1)\pi\}_{p \in \mathbb{Z}},$$

which is a countable union of straight lines. Figure 2 shows the graphs of $\lambda_{\pm}(\cdot)$ for $v_0 = 0$, $v_1 = 2$, with the dashed lines indicating the level sets at the edges of the gap $[0, 2]$.

Remark 7.1. This example seems to be one of the simplest possible 2D diatomic tight binding models. We believe that it should be known to the experts in solid state physics. We could not, however, find it in the literature, which is the reason why we discuss it in detail.

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